```
HITS AT: 1-3, 4-10
 L7
    ANSWER 9 OF 29 REGISTRY COPYRIGHT 1998 ACS
 RN
   120618-88-4 REGISTRY
 FS PROTEIN SEQUENCE
 SQL 10
NTE cyclic
    modified
            ----- location -----
                                  description
 _____
uncommon
            Orn-5
modification Orn-5
                              undetermined modification
 SEQ 1 NQYVXLFPWF
        ========
HITS AT: 1-3, 4-10
   ANSWER 10 OF 29 REGISTRY COPYRIGHT 1998 ACS
L7
RN 120602-98-4 REGISTRY
FS PROTEIN SEQUENCE
SQL 10
NTE cyclic
   modified
            ----- location ----- description
uncommon Orn-5 -
modification Tyr-3 -
                           iodo<2; I>
SEQ 1 NQYVXLFPWF
       ========
HITS AT: 1-3, 4-10
L7
   ANSWER 11 OF 29 REGISTRY COPYRIGHT 1998 ACS
   42002-32-4 REGISTRY
RN
FS
   PROTEIN SEQUENCE
SQL 10
NTE cyclic
  modified
----- location -----
                                  description
uncommon Orn-5 - - phenylmethyl<Bzl>
modification Orn-5 - (phenylmethoxy)carbonyl<Z>
SEQ
HITS AT: 1-3, 4-10
  ANSWER 12 OF 29 REGISTRY COPYRIGHT 1998 ACS
L7
   28382-58-3 REGISTRY
RN
FS
   PROTEIN SEQUENCE
SQL 10
NTE cyclic
  modified
_______
type
           ----- location -----
                                  description
```

SEQ 1 NQYVXLFPFF

```
uncommon Orn-5 - - undetermined modification
SEQ 1 NQFVXLFPFF
       ========
HITS AT: 1-3, 4-10
  ANSWER 13 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN 28343-15-9 REGISTRY
DR 27562-00-1
FS PROTEIN SEQUENCE
SQL 10
NTE cyclic
   modified
               ----- location ----- description
       ______
uncommon Orn-5
modification -
                           undetermined modification
SEQ 1 NQYVXLFPWW
       ========
HITS AT: 1-3, 4-10
L7
  ANSWER 14 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN
  28343-14-8 REGISTRY
FS
  PROTEIN SEQUENCE
SQL 10
NTE cyclic
   modified
----- location -----
                              description
------
uncommon Orn-5 modification Orn-5
                    -
                        (phenylmethoxy) carbonyl < Z >
------
SEQ 1 NQYVXLFPWW
      ========
HITS AT: 1-3, 4-10
L7
  ANSWER 15 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN
  28334-51-2 REGISTRY
FS
  PROTEIN SEQUENCE
SQL 10
NTE cyclic
  modified
______
          ----- location ----- description
 uncommon Orn-5 -
modification Orn-5 -
                 -
                       (phenylmethoxy)carbonyl<Z>
    -----
SEQ 1 NQFVXLFPFF
      ========
HITS AT: 1-3, 4-10
L7
  ANSWER 16 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN
  27805-48-7 REGISTRY
FS
  PROTEIN SEQUENCE
SQL 10
```

```
NTE cyclic
   modified
   -----
          ----- location -----
                           description
 uncommon Orn-5 modification -
 modification
                        undetermined modification
 -----
SEQ
   1 NQYVXLFPWF
      ========
HITS AT: 1-3, 4-10
   ANSWER 17 OF 29 REGISTRY COPYRIGHT 1998 ACS
   27783-64-8 REGISTRY
  PROTEIN SEQUENCE
SQL 10
NTE cyclic
   modified
         ----- location -----
                           description
______
uncommon Orn-5 -
modification Orn-5 -
                       (phenylmethoxy)carbonyl<Z>
SEQ 1 NQYVXLFPWF
      ========
HITS AT: 1-3, 4-10
  ANSWER 18 OF 29 REGISTRY COPYRIGHT 1998 ACS
L7
RN 23619-01-4 REGISTRY
FS
  PROTEIN SEQUENCE
SQL 10
NTE cyclic
------
         ----- location -----
                          description
uncommon
        Orn-5
  ______
SEQ 1 NQYVXLFPYY
     ========
HITS AT: 1-3, 4-10
  ANSWER 19 OF 29 REGISTRY COPYRIGHT 1998 ACS
  23512-44-9 REGISTRY
RN
FS
  PROTEIN SEQUENCE
SQL 10
NTE cyclic
______
         ----- location ----- description
-
uncommon
        Orn-5
-----
SEQ 1 NQYVXLFPYF
     ========
HITS AT: 1-3, 4-10
L7
  ANSWER 20 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN
  19716-16-6 REGISTRY
DR 11005-77-9
```

FS PROTEIN SEQUENCE

SQL 10

```
NTE cyclic
 ------
           ----- location -----
                             description
 uncommon
          Orn-5
 -----
 SEQ 1 NOWVXLFPWW
       ========
 HITS AT: 1-3, 4-10
L7
   ANSWER 21 OF 29 REGISTRY COPYRIGHT 1998 ACS
   19659-43-9 REGISTRY
FS
   PROTEIN SEQUENCE
SQL 10
NTE cyclic
     -----
          ----- location ----- description
______
uncommon Orn-5
SEQ 1 NQYVXIFPFF
      ========
HITS AT: 1-3, 4-10
L7
  ANSWER 22 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN
  19659-41-7 REGISTRY
FS PROTEIN SEQUENCE
SQL 10
NTE cyclic
_____
         ----- location -----
                            description
------
uncommon
       Orn-5
______
SEQ 1 NQFVXLFPFF
      ========
HITS AT: 1-3, 4-10
L7
  ANSWER 23 OF 29 REGISTRY COPYRIGHT 1998 ACS
  6676-11-5 REGISTRY
RN
FS
   PROTEIN SEQUENCE
SQL 10
NTE cyclic
   modified
-----
         ----- location ----
                            description
 -
uncommon Orn-5 modification Orn-5
                _
                      (phenylmethoxy)carbonyl<Z>
------
SEQ 1 NQYVXLFPFF
      ========
HITS AT: 1-3, 4-10
  ANSWER 24 OF 29 REGISTRY COPYRIGHT 1998 ACS
L7
RN
  6060-42-0 REGISTRY
FS
  PROTEIN SEQUENCE
SQL 10
NTE cyclic
  modified
```

type	loc	ation	description
uncommon modification	Orn-5 -	- -	undetermined modification
	=======		
HITS AT: 1-	-3, 4-10		
RN 3991-13- FS PROTEIN SQL 10 NTE cyclic	SEQUENCE		1998 ACS
type	loc	ation	description
uncommon	Orn-5	-	-
SEQ 1 NG			
HITS AT: 1-	-3, 4-10		
RN 3252-29- DR 11018-02 FS PROTEIN SQL 10 NTE cyclic	SEQUENCE		1998 ACS
type	loc	ation	description
uncommon	Orn-5	-	-
SEQ 1 NÇ	 _YVXLFPWW ========		
HITS AT: 1-	-3, 4-10		
		TRY COPYRIGHT	1998 ACS
type	loc	ation	description
uncommon			-
SEQ 1 NÇ			
HITS AT: 1-	-3, 4-10		
RN 1111-57-	28 OF 29 REGIS -5 REGISTRY SEQUENCE	TRY COPYRIGHT	1998 ACS
type	loc	 ation	description
	-		

uncommon Orn-5 SEQ 1 NQYVXLWPWF ======== HITS AT: 1-3, 4-10 L7 ANSWER 29 OF 29 REGISTRY COPYRIGHT 1998 ACS RN 865-28-1 REGISTRY FS PROTEIN SEQUENCE SQL 10 NTE cyclic ______ ----- location ----- description uncommon Orn-5 - -______ 1 NQYVXLFPWF ======== HITS AT: 1-3, 4-10

```
========
 HITS AT: 1-3, 4-10
 L7
   ANSWER 5 OF 29 REGISTRY COPYRIGHT 1998 ACS
   182351-66-2 REGISTRY
 RN
 FS PROTEIN SEQUENCE; STEREOSEARCH
 SQL 10
NTE cyclic
   modified (modifications unspecified)
 ------
         ----- location -----
                            description
 uncommon
          Orn-5
stereo Tyr-7
                         D
             -----
HITS AT:
      1-3, 4-10
  ANSWER 6 OF 29 REGISTRY COPYRIGHT 1998 ACS
L7
RN 147344-92-1 REGISTRY
FS PROTEIN SEQUENCE
SQL 10
NTE cyclic
-----
         ----- location -----
                            description
uncommon
SEQ 1 NQWVXLFPFF
      ========
HITS AT: 1-3, 4-10
L7
  ANSWER 7 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN
  147316-75-4 REGISTRY
  PROTEIN SEQUENCE
FS
SQL 10
NTE cyclic
----- location ----- description
uncommon
         Orn-5
------
SEQ 1 NQWVXLFPWF
      ========
HITS AT: 1-3, 4-10
   ANSWER 8 OF 29 REGISTRY COPYRIGHT 1998 ACS
RN
   136207-54-0 REGISTRY
FS
   PROTEIN SEQUENCE
SQL 10
NTE cyclic
  modified
----- location ----- description
uncommon Orn-5
modification Tyr-3
modification Orn-5
              undetermined modification(phenylmethoxy)carbonyl<Z>
```

SEQ 1 NDWVXLYPFF

	OF 29 REGISTRY -5 REGISTRY EQUENCE; STERE	RY COPYRIGHT	' 1998 ACS
type	loca	ation	description
uncommon modification modification	Orn 5		-
SEQ 1 NDW			
	OF 29 REGISTR -4 REGISTRY		1998 ACS
type	loca	tion	description
uncommon	Orn-5	-	-
SEQ 1 NDW\	VITEME		
HITS AT: 1-3, L7 ANSWER 3 C RN 202752-12- FS PROTEIN SE SQL 10	 4-10 OF 29 REGISTR -3 REGISTRY CQUENCE; STERE		1998 ACS
HITS AT: 1-3, L7 ANSWER 3 C RN 202752-12- FS PROTEIN SE SQL 10 NTE cyclic	4-10 DF 29 REGISTR 3 REGISTRY CQUENCE; STERE	OSEARCH	description
HITS AT: 1-3, L7 ANSWER 3 C RN 202752-12- FS PROTEIN SE SQL 10 NTE cyclic type	4-10 DF 29 REGISTR 3 REGISTRY CQUENCE; STERE	OSEARCH	description
HITS AT: 1-3, L7 ANSWER 3 C RN 202752-12- FS PROTEIN SE SQL 10 NTE cyclic type uncommon SEQ 1 NDYV ==== HITS AT: 1-3, L7 ANSWER 4 O RN 182422-45-	4-10 OF 29 REGISTRY QUENCE; STERE loca Orn-5 XLYPFF	OSEARCH tion	description
HITS AT: 1-3, L7 ANSWER 3 C RN 202752-12- FS PROTEIN SE SQL 10 NTE cyclic type Uncommon SEQ 1 NDYV === HITS AT: 1-3, L7 ANSWER 4 O RN 182422-45- FS PROTEIN SE SQL 10	4-10 OF 29 REGISTRY QUENCE; STERE Orn-5 XLYPFF ===== 4-10 F 29 REGISTRY QUENCE; STEREO	OSEARCH tion COPYRIGHT DSEARCH	description 1998 ACS description

```
L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 1998 ACS
```

- AN 1993:209087 CAPLUS
- DN 118:209087
- TI Characterization of the tyrocidine and gramicidin fractions of the tyrothricin complex from Bacillus brevis using liquid chromatography and mass spectrometry
- AU Tang, Xue Jun; Thibault, Pierre; Boyd, Robert K.
- CS Inst. Mar. Biosci., Natl. Res. Counc., Halifax, NS, B3H 3Z1, Can.
- SO Int. J. Mass Spectrom. Ion Processes (1992), 122, 153-79 CODEN: IJMPDN; ISSN: 0168-1176
- DT Journal
- LA English
- L8 ANSWER 2 OF 2 CAPLUS COPYRIGHT 1998 ACS
- AN 1993:209086 CAPLUS
- DN 118:209086
- TI An investigation of the tyrothricin complex by tandem mass spectrometry
- AU Barber, M.; Bell, D. J.; Morris, M. R.; Tetler, L. W.; Monaghan, J. J.; Morden, W. E.; Bycroft, B. W.; Green, B. N.
- CS Dep. Chem., UMIST, Manchester, M60 1QD, UK
- SO Int. J. Mass Spectrom. Ion Processes (1992), 122, 143-51 CODEN: IJMPDN; ISSN: 0168-1176
- DT Journal
- LA English
- => d all 1-

YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

- L8 ANSWER 1 OF 2 CAPLUS COPYRIGHT 1998 ACS
- AN 1993:209087 CAPLUS
- DN 118:209087
- Characterization of the tyrocidine and gramicidin fractions of the tyrothricin complex from Bacillus brevis using liquid chromatography and mass spectrometry
- AU Tang, Xue Jun; Thibault, Pierre; Boyd, Robert K.
- CS Inst. Mar. Biosci., Natl. Res. Counc., Halifax, NS, B3H 3Z1, Can.
- SO Int. J. Mass Spectrom. Ion Processes (1992), 122, 153-79 CODEN: IJMPDN; ISSN: 0168-1176
- DT Journal
- LA English
- CC 10-1 (Microbial, Algal, and Fungal Biochemistry)
 Section cross-reference(s): 9, 26
- The tyrothricin peptide complex, isolated from the fermn. broth of Bacillus brevis, is comprised of a basic fraction of cyclic decapeptides (the tyrocidines) and a neutral fraction composed of linear peptides (the gramicidins). Previously, 5 cyclic compds. (tyrocidines A-E) had been characterized by classical chem. procedures, and an addnl. 5 by M. Barber et al. (1992), who employed tandem mass spectrometric anal. of the crude mixt., together with an interpretative strategy based upon mass shifts related to simple amino acid substitutions. In the present work, initial profiling of the tyrothricin complex, using reverse phase liq. chromatog. (HPLC) coupled directly to tandem mass spectrometry via an ionspray interface, showed that the mixt. is extremely complex. Semi-preparative HPLC provided 32 fractions, some of which were still mixts., amenable to anal. by tandem mass spectrometry using

```
ANSWER 1 OF 2 CAPLUS COPYRIGHT 1998 ACS
L8
    1993:209087 CAPLUS
AN
     118:209087
DN
     Characterization of the tyrocidine and gramicidin fractions of the
ΤI
     tyrothricin complex from Bacillus brevis using liquid chromatography
     and mass spectrometry
     Tang, Xue Jun; Thibault, Pierre; Boyd, Robert K.
ΑU
     Inst. Mar. Biosci., Natl. Res. Counc., Halifax, NS, B3H 3Z1, Can.
CS
     Int. J. Mass Spectrom. Ion Processes (1992), 122, 153-79
SO
     CODEN: IJMPDN; ISSN: 0168-1176
     Journal
DT
     English
LΑ
     10-1 (Microbial, Algal, and Fungal Biochemistry)
CC
     Section cross-reference(s): 9, 26
     The tyrothricin peptide complex, isolated from the fermn. broth of
AB
     Bacillus brevis, is comprised of a basic fraction of cyclic
     decapeptides (the tyrocidines) and a neutral fraction composed of
     linear peptides (the gramicidins). Previously, 5 cyclic compds.
     (tyrocidines A-E) had been characterized by classical chem.
     procedures, and an addnl. 5 by M. Barber et al. (1992), who employed
     tandem mass spectrometric anal. of the crude mixt., together with an
     interpretative strategy based upon mass shifts related to simple
     amino acid substitutions. In the present work, initial profiling of
     the tyrothricin complex, using reverse phase liq. chromatog. (HPLC)
     coupled directly to tandem mass spectrometry via an ionspray
     interface, showed that the mixt. is extremely complex.
     Semi-preparative HPLC provided 32 fractions, some of which were
     still mixts., amenable to anal. by tandem mass spectrometry using
     the doubly-protonated peptide precursors produced by ionspray
     ionization. In this way the 10 previously known tyrocidines were
     confirmed, and structures of an addnl. 18 cyclic variants
     established with only minor uncertainties (e.g. present techniques
     could not distinguish Ile from Leu). Six linear gramicidins were
     known previously, and were confirmed in the present work. In addn.,
     3 previously unknown variants, of the Vall-gramicidins A, B and C,
     were discovered, in which the ethanolamide residue at the C-terminus
     is replaced by a propanolamide residue.
     Bacillus tyrocidine gramicidin fraction HPLC spectrometry;
     tyrothricin complex mass spectrometry liq chromatog
     Bacillus brevis
        (gramicidin and thyrocidine from, isolation and structure of)
                1404-88-2, Tyrothricin
                                        1405-97-6, Gramicidin
     865-28-1
                                                     5536-03-8
                 3252-29-7
                           4419-81-2
                                         4422-52-0
     1481-70-5
                                                     19659-42-8
                 8011-61-8, Tyrocidine 19659-41-7
     6377-07-7
                                                        147316-74-3
                               64765-31-7 147316-73-2
     19716-16-6
                 58442-65-2
     147316-75-4 147344-92-1
     RL: BIOL (Biological study)
```

(from Bacillus brevis, isolation and structure of)

the doubly-protonated peptide precursors produced by ionspray ionization. In this way the 10 previously known tyrocidines were confirmed, and structures of an addnl. 18 cyclic variants established with only minor uncertainties (e.g. present techniques could not distinguish Ile from Leu). Six linear gramicidins were known previously, and were confirmed in the present work. In addn., 3 previously unknown variants, of the Vall-gramicidins A, B and C, were discovered, in which the ethanolamide residue at the C-terminus is replaced by a propanolamide residue. Bacillus tyrocidine gramicidin fraction HPLC spectrometry; tyrothricin complex mass spectrometry liq chromatog Bacillus brevis (gramicidin and thyrocidine from, isolation and structure of) 1404-88-2, Tyrothricin 1405-97-6, Gramicidin 865-28-1 3252-29-7 4419-81-2 4422-52-0 5536-03-8 1481-70-5 19659-41-7 8011-61-8, Tyrocidine 19659-42-8 6377-07-7 64765-31-7 147316-73-2 147316-74-3 19716-16-6 58442-65-2 147316-75-4 147344-92-1 RL: BIOL (Biological study) (from Bacillus brevis, isolation and structure of) ANSWER 2 OF 2 CAPLUS COPYRIGHT 1998 ACS 1993:209086 CAPLUS 118:209086 An investigation of the tyrothricin complex by tandem mass spectrometry Barber, M.; Bell, D. J.; Morris, M. R.; Tetler, L. W.; Monaghan, J. J.; Morden, W. E.; Bycroft, B. W.; Green, B. N. Dep. Chem., UMIST, Manchester, M60 1QD, UK Int. J. Mass Spectrom. Ion Processes (1992), 122, 143-51 CODEN: IJMPDN; ISSN: 0168-1176 Journal English 10-1 (Microbial, Algal, and Fungal Biochemistry) Section cross-reference(s): 9, 26 Tandem mass spectrometry has been shown to be a powerful technique for detg. the structures of biol. compds. This paper details the mass spectrometric methods employed to characterize the structural variations found within a mixt. of cyclic decapeptides, tyrothricin, produced by the bacterium Bacillus brevis. Bacillus tyrothricin complex tandem mass spectrometry Nomenclature, new natural products (tryptocidin A) Nomenclature, new natural products (tryptocidin B) Nomenclature, new natural products (tryptocidin C) Nomenclature, new natural products (tryptocidin C1) Nomenclature, new natural products (tyrocidin A1) Nomenclature, new natural products (tyrocidin B1) Nomenclature, new natural products (tyrocidin C) Bacillus brevis (tyrothricin complex from, tandem mass spectrometry anal. of) 1404-88-2, Tyrothricin 1481-70-5 3252-29-7 865-28-1 19716-16-6 147316-73-2 147316-74-3 147316-75-4 19659-42-8 147344-92-1

(from Bacillus brevis, tandem mass spectrometry anal. of)

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RL: BIOL (Biological study)